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Coordination chemistry of cerium and neptunium catecholates in aqueous solution

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Host: Dr. Linfeng Rao

ABSTRACT

Both the EXAFS (Extended X-ray Absorption Fine Structure) and XANES (X-ray Absorption Near Edge Structure) regions of an XAS spectrum have been proven to be useful in the determination of species in solution. EXAFS has been used to help elucidate the structures of Ce(III), Ce(IV), Np(V) and Np(VI) complexes with the ligands catecholate and Tironate (proligand = Tiron or disodium 4,5-dihydroxy-*m*-benzenedisulfonate) at high pH. An average coordination number of 5 (± 1) was obtained from the data for the Ce-Tironate solutions, which is unusually low. This has been attributed to Atomic XAFS and will be discussed. The first EXAFS analysis of Np with catecholate and Tironate ligands in aqueous solution will also be reported, with evidence to support the existence of both monomeric and dimeric species in solution.